Ideal gas provides q-entropy

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The thermodynamical probability for an ideal gas having a given energy, E, and the conditional probability for a part of an ideal gas having another energy, E_1, are considered both in the traditional way and in a factorizing setting. The latter delivers the q-entropy formulas of Rényi and Tsallis. The factorizing quantity and the corresponding q-entropy is obtained for both types of probabilities. Finally perspectives for generalizations to systems with energy- or entropy-dependent heat capacity are discussed.

MICROCANONICAL EQUATION OF STATE FOR AN IDEAL GAS

In this paper we point out how the q-entropy [1–7] emerges in terms of the traditional thermodynamics of the ideal gas. First we concentrate on the classical ideal gas[8] defined by an equation of state with constant heat capacity [9, 10], then we consider possible generalizations of this idea to include more complex systems, having a linear heat capacity – entropy relation.

In the statistical mechanics the ideal gas is viewed as a mechanical system of N particles completely described by their kinetic energy. The energy-momentum relation, $E(\vec{p})$, translates the classical uniform phase space distribution to a state density $\rho(E) = d\Gamma/dE$. In particularly simple cases, like the non-relativistic kinetic energy of massive particles, $E = \vec{p}^2/2m$, the state density has the form $\rho(E) \propto V E^f$.

Fixing the total energy as a constant sum of the individual energies leads to a uniform occupation of a spherical shell in the $2ND$-dimensional phase space. The volume and total energy scaling of such a shell-volume is easy to obtain at a fixed particle number, N:

$$W_N(E) = e^{S(E)} = \int \prod_{j=1}^{N} d\Gamma_j \, \delta\left(E - \sum_{i=1}^{N} E_i\right) \propto V^N E^{fN-1} \tag{1}$$

with $d\Gamma = dV d^D p/(2\pi\hbar)^D$ and $f = D/2$ in D dimensions. Boltzmann has suggested that the a priori equally probable states are realized with a relative frequency of $P = 1/W = e^{-S(E)}$ in a huge number of observations. $1/W$ is traditionally called "thermodynamical probability". From here the entropy, $S = \ln W$ [11] (with unit Boltzmann constant $k_B = 1$) is given as

$$S(E, V, N) = S_0(N) + N \ln V + (fN - 1) \ln E. \tag{2}$$

Such an equation of state leads to an energy and volume independent heat capacity, $C_{V,N} = fN - 1$, for a fixed particle number, N [11]. From now on we simplify the discussion to fixed volume and particle number, dealing with the equation of state in form of a single $S(E)$ relation. Primes denote then derivatives with respect to the corresponding single argument.

We consider a class of equations of state with *constant heat capacity*. In this case $1/C := -S''(E)/S'(E)^2 = 1/C_0$ is energy independent and the differential equation can be solved for $S(E)$. Its first integral becomes the temperature $T = 1/S'(E) = T_0 + E/C_0$, with T_0 being an integration constant. Its physical meaning is associated to the minimal energy, $E_0 = C_0 T_0$, belonging to $W(E_0) = 1$. The ideal gas temperature is in general a linear function of the energy E. The second integration leads to the general microcanonical equation of state with constant heat capacity:

$$S(E) = C_0 \ln\left(1 + \frac{E}{C_0 T_0}\right) + S_0. \tag{3}$$

Counting the energy E relative to the state with minimal classical energy, $E = 0$, we require $S(0) = 0$ according to the third law of thermodynamics. This fully defines an ideal gas. The coefficients C_0 and T_0 may differ from problem to problem. We note, however, that T_0 is never exactly zero in real systems, as long as the entropy $S(E)$ is non-negative.

The exponentiated entropy upon eq.(3) with $S_0 = 0$

$$W = e^{S(E)} = \left(1 + \frac{E}{C_0 T_0}\right)^{C_0} \tag{4}$$

delivers the thermodynamical probability of having energy E of a system. For an *isolated* system having energy E_1 therefore the microcanonical probability is [8]

$$P(E_1) = e^{-S(E_1)} = \left(1 + \frac{E_1}{C_0 T_0}\right)^{-C_0}. \tag{5}$$

On the other hand the conditional probability of a *subsystem* having energy E_1 while the total energy is fixed to E becomes:

$$P^*(E_1|E) := \frac{W(E - E_1)}{W(E)} = \left(1 - \frac{E_1}{C_0 T}\right)^{C_0} \tag{6}$$

with $T = T_0 + E/C_0$. Note that – after some algebra – in the denominator T occurs in place of T_0. In the infinite N limit an exponential distribution emerges,

$$P^*(E_1|E) \longrightarrow e^{-E_1/T}. \tag{7}$$

This result is frequently quoted as the "equivalence of the canonical and microcanonical statistics in the thermodynamical limit". It, however, does not hold for all arbitrary ratios of fluctuations in arbitrary systems [12–18]. The finite ideal gas has been studied and showed to lead to a density of states in the subsystem which interpolates between microcanonical and canonical distributions as the heat capacity of the reservoir part grows from zero to infinity [19].

In finite ideal gas the conditional probability for a subsystem with a given energy and the Boltzmannian thermodynamical probability vastly differ,

$$P^*(E_1|E) = e^{S(E-E_1)-S(E)} \neq e^{-S(E_1)} = P(E_1), \quad (8)$$

basically due to the *non-additivity* of the microcanonical entropy. While the energy is additive, the ideal gas entropy is not.

It is a relevant question which probability influences experimental observations. Regarding a long term observation of N particles with total energy E, a single particle has energy E_1 with the frequency $P^*(E_1|E)$. Here, however, one supposes that the *observed particle remains in the system* for infinitely many consecutive observations. If the *particle is taken out* after each observation, then the energy and number of particles both diminish during detection. Then to observe first an energy E_1 out of E and then an energy E_2 out of $E - E_1$ etc. delivers

$$P^*(E_1|E)P^*(E_2|E-E_1)\dots P^*(E_N|E-E_1-\dots-E_{N-1}) =$$

$$= \frac{W(E-E_1)}{W(E)} \frac{W(E-E_1-E_2)}{W(E-E_1)} \cdots \frac{W(0)}{W(E-\dots-E_{N-1})}$$

$$= \frac{1}{W(E)} = P(E), \quad (9)$$

due to the steady cancellation of W-factors in the chain of ratios. This points out the physical meaning of the thermodynamical probability, $1/W$. So the observation of any partition of the initial energy E by a decay is equally probable.

q-ENTROPY OF THE IDEAL GAS

A possible improvement towards mathematical beauty is achieved if factorization is performed. This procedure can be applied both to the thermodynamical (5) and conditional (6) probabilities. In this way the part of an ideal gas becomes itself an ideal gas. Generalizing Boltzmann's idea one seeks for a probability, based on a given function of the original entropy, $K(S)$. Considering

$$P_K(E) = e^{-K(S(E))}, \quad (10)$$

one uses an additive function of the original entropy, a "formal logarithm" [20, 21]. Since we assume additivity of the energy, *this can only be a linear expression of E.* By using the functional form inverting the ideal gas equation of state with constant heat capacity, eq.(3) exactly, we have

$$K(S) = \lambda E + \mu = \lambda C_0 T_0 \left(e^{S/C_0} - 1 \right) + \mu. \quad (11)$$

Satisfying the natural requirement of $K(S) \approx S$ for small S one fixes $K(0) = 0$ and $K'(0) = 1$. This determines the linearity parameters as $\mu = 0$ and $\lambda = 1/T_0$. We get

$$K(S) = C_0 \left(e^{S/C_0} - 1 \right). \quad (12)$$

It is important to realize that this result is *independent of the integration constant T_0.* Using this construction $P_K^*(E_1) = P_K(E_1)$. Obviously $K(S(E_1)) + K(S(E - E_1)) = K(S(E))$; the finite ideal gas entropy is K-*additive* and the factorization is done.

We repeat this procedure for the conditional probability. Seeking for an additive function of $X = -\ln P^*$ we consider

$$K^*(-\ln P^*(E_1)) = \lambda E_1 + \mu. \quad (13)$$

Inverting eq.(6) we obtain

$$K^*(X) = \lambda C_0 T \left(1 - e^{-X/C_0} \right) + \mu. \quad (14)$$

With the natural conditions $K^*(0) = 0$ and $(K^*)'(0) = 1$ finally we arrive at

$$K^*(X) = C_0 \left(1 - e^{-X/C_0} \right). \quad (15)$$

It is noteworthy that this result is independent of the temperature, T. The factorizing 'star'-quantity becomes

$$P_{K^*}(E_1) := e^{-K^*(-\ln P^*(E_1))} = e^{-E_1/T}. \quad (16)$$

For considering an *ensemble* of systems of each kind we average the above additive quantities, K and K^*, over the corresponding probabilities, P and P^*. The traditional way, derivable from Boltzmann's permutation formula using the Stirling formula for the logarithm of the large factorials, delivers

$$S_{\text{Gibbs}} = \sum_i P_i(-\ln P_i). \quad (17)$$

The idea behind, however, is based on the additivity of the terms, on the independence of the probabilities P_i being in a state of E_i. This concept must hold for physical situations where each E_i energy occurs *independently.* On the other hand if a system of finite total energy E has subsystems with energies E_i, then one observes *correlated* probabilities. The above Gibbs-formula (17) fails to be correct. Then only the really independent, factorizing

K-probabilities are allowed to be considered and instead of the Boltzmann-entropy, the $K(S_i)$ quantities have to be added. We obtain

$$K(S) = \sum_i P_i K(-\ln P_i) \qquad (18)$$

for the thermodynamical and

$$K^*(X) = \sum_i P_i^* K^*(-\ln P_i^*) \qquad (19)$$

for the conditional probabilities and corresponding formal entropies.

First we consider the additive entropy based on the thermodynamical probability. Applying our result (12) we arrive at

$$K(S) = C_0 \sum_i P_i(e^{(-\ln P_i)/C_0} - 1). \qquad (20)$$

By using $q = 1 - 1/C_0$ (with C_0 being the heat capacity of the isolated system) this expression takes the form of Tsallis q-entropy:

$$K(S) = \frac{1}{1-q} \sum_i \left(P_i^q - P_i\right). \qquad (21)$$

It is noteworthy that S becomes now the Rényi formula:

$$S = \frac{1}{1-q} \ln \sum_i P_i^q. \qquad (22)$$

Next we consider the additive entropy based on the conditional probability. Based on (15) we obtain

$$K^*(X) = C_0 \sum_i P_i^*(1 - e^{(\ln P_i^*)/C_0}) \qquad (23)$$

with $X = S(E) - S(E - E_1)$. Using now $q^* = 1 + 1/C_0$ (with C_0 being the heat capacity of the reservoir) this expression also takes the form of a Tsallis formula, but with a dual parameter $q^* = 2 - q$:

$$K^*(X) = \frac{1}{1-q^*} \sum_i \left((P_i^*)^{q^*} - P_i^*\right). \qquad (24)$$

Again the original entropy factor, $X = S(E) - S(E - E_1)$ is given as a Rényi formula:

$$X = \frac{1}{1-q^*} \ln \sum_i (P_i^*)^{q^*}. \qquad (25)$$

This relation between thermodynamical and conditional probabilities for an ideal gas show unexpectedly a new facet of the "q-duality" [7].

FORMALLY CANONICAL TREATMENT

The factorizing quantities, P_K and P_{K^*}, are exponential functions of the additive energy variables, they formally looks "canonical", c.f. eq.(16). However, please note that $T_0 \neq T$. For positive heat capacity ("normal") physical systems $T > T_0$. This is the basic reason why cut power-law fits to observed spectra give a smaller slope parameter extrapolated to zero energy than direct fits to an exponential function [22–31]. Supporting these ensemble-entropy formulas by conditions of probability normalization and average energy one arrives at the formal *K-canonical* principle

$$\left(\sum_i P_i K(-\ln P_i) - K(S(E))\right) - \alpha \left(\sum_i P_i - 1\right)$$
$$- \beta \left(\sum_i P_i E_i - \langle E \rangle\right) = \max. \qquad (26)$$

for a generic P_i distribution, either conditional or thermodynamical. This view already includes factorization and is the form compatible with a temperature definition independent of the subsystem-rest division [33, 34].

Thus we arrive at the Tsallis and Rényi formulas for the q-entropy either with $q = 1 - 1/C_0$ or with $q^* = 1 + 1/C_0$ depending on which probability is observed: In the former case the isolated systems' microcanonical probability, in the second case the conditional finite subsystem – finite reservoir probability. It is a curious fact that these, in their origin microcanonical probabilities can be obtained from a formally canonical treatment by the variational principle (26). The formally canonical distribution, constrained by the average energy and probability normalization is given by the stationary point of eq.(26) with respect to all P_i-s:

$$P_{\mathrm{K-cano}}(E_i) = \left(1 + \frac{1 + \alpha + \beta E_i}{C_0 - 1}\right)^{-C_0}. \qquad (27)$$

in the case $q = 1 - 1/C_0$ (5). The single particle energy distribution in an undisturbed N-particle ideal gas is obtained by using $q^* = 1 + 1/C_0$ on the other hand (6):

$$P_{\mathrm{K*-cano}}^*(E_i) = \left(1 - \frac{1 + \alpha + \beta E_i}{C_0 + 1}\right)^{C_0}. \qquad (28)$$

Usually, for a sensible positive average energy, α and β are positive, so the *K-canonical* probability distribution is of one plus energy on a negative power type, going above the exponential. This exactly reconstructs the thermodynamical probability for a fixed number ideal gas. The K^*-*canonical* distribution behaves opposite.

GENERALIZATION

There is a general lesson from the above. Considering an additive function of a non-additive entropy formula while the energy is kept additive *can only be* an expression proportional to the energy: $K(S(E)) = E/T_0$. With other words, the second derivative of $K(S(E))$ with respect to the energy vanishes: $\frac{\mathrm{d}^2}{\mathrm{d}E^2}K(S(E)) = 0$. Applying the chain rule, this is equivalent to

$$\frac{K''(S)}{K'(S)} = -\frac{S''(E)}{S'(E)^2} = \frac{1}{C}, \qquad (29)$$

pointing out the central role of the heat capacity by such constructions. There is a general formal solution, $K(S) = \int \exp(\int dS/C(S))dS$. Now the first derivative of $K(S(E))$ with respect to the energy, E, is independent of the energy. This makes it possible to satisfy the zeroth law of thermodynamics universally; the temperature of a subsystem is independent of the energy of the same subsystem. This *universal thermostat independence* (UTI) principle[33] allows to define a temperature in the microcanonical analysis.

For an ideal gas with constant number of particles, N, also the heat capacity, $C_{V,N}$, is constant. After abandoning this fixing more general connections, $C(S)$, should be taken into account even for ideal gases. Physically important examples are black body radiation, extensible to models with bag constant, where $C = 3S$, and simple black hole horizon thermodynamics with $C = -2S$. In these cases N is not a basic thermodynamical variable, in the second case even V is missing. We present here the corresponding formulas for the linear class of equations of state, $C(S) = C_0 + C_1 S$. In this case the equation of state integrates to

$$S(E) = \frac{C_0}{C_1}\left[\left(1 + \frac{C_1+1}{C_0 T_0}E\right)^{\frac{C_1}{C_1+1}} - 1\right]. \qquad (30)$$

One obtains

$$K^*(X) = \frac{C}{C_1}\sum_i P_i^* \frac{1}{q_1}\left[1 - \left(1 + \frac{C_1}{C}\ln P_i^*\right)^{q_1}\right] \quad (31)$$

with $q_1 = 1 + 1/C_1$ and $C = C_0 + C_1 S$ for the entropy formula (19) associated to the conditional (finite-canonical) probability. For $C \to \infty$ the Gibbs formula (17), for $C_1 \to 0$ the Tsallis formula (24) arises. An exploration of the potential of these formulas, in particular for $C_0 = 0$, is referred to a future work.

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